ELASTIC RESONANCE IN ELECTRON-HYDROGEN SCATTERING

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ABSTRACT. The singlet s-wave phase shifts in the elastic scattering of slow electrons by atomic hydrogen have been calculated in the energy range below the threshold for the excitation of second quantum level (10.2 ev) by Hulthén's variational method. The exchange effect has been allowed for and the polarisation effect has been considered through the process of virtual excitation to 2S and $2P_0$ levels. We obtain a resonance level at 9.55 ev energy, which agrees favourably with the recent experimental findings and the results of other theoretical calculations.

INTRODUCTION

Several experiments have been carried out on slow electron scattering by atomic hydrogen. Schulz (1964), Kleinpoppen *et al.* (1965) and McGowan *et al,* (1964) have found experimentally elastic resonances below the threshold for excitation of electronic states of atomic hydrogen.

A number of theoretical investigations has been made on $\bar{e}-H$ collision problem which has been discussed in our previous work (1965), where we have dealt with the same problem by Hulthén's variational method considering the polarisation effect through the virtual excitation to $2S$ and $2P_0$ level but neglecting the exchange effect. Here in the present paper, we have used the same variational method and have considered the exchange effect by explicitly antisymmetrising the wavefunction with respect to the atomic and incoming electrons, the polarisation effect has been taken into account in the same way as in our previous work (1965) so as to include virtual excitation to $2S$ and $2P_0$ levels. Recently, Geltman (1965) has applied variational method to investigate the $\bar{e}-H$ scattering with a particular choice of trial function so as to take into consideration the virtual excitation to higher excited states and has obtained very narrow resonances at electron energies below the first inelastic threshold. Burke and Taylor (1966) also have carried out close coupling calculations including correlation in their trial function on the resonances in $\bar{e}-H$ scattering.

Our calculations for singlet S-wave phase shifts indicate a resonance at an energy of 9.55 ev, which agrees satisfactorily with the experimental findings of Schulz (1964), Kleinpoppen *et al.* (1965), McGowan *et al.* (1965) and also with the results of other theoretical calculations.

THEORY

The wavefunction $\psi(r_1, r_2)$ of the system of two electrons moving in the field of a proton satisfies the wave equation $(H-E)\psi(r_1, r_2) = 0$ ... (1)

with
$$H = -\frac{\Delta_1^2}{2} - \frac{\Delta_2^2}{2} - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}}$$

in atomic units (i.e. $e = m = \hbar = 1 = a_0$), here r_1 and r_2 are the co-ordinates of the atomic and incoming electrons, relative to the proton and r_{12} is their mutual distance.

Since the total wave function of the system of two electrons must be anti-symmetric for exchange of their space and spin co-ordinates,
we therefore choose for ψ the forms

$$\psi^{\pm}(r_1, r_2) = \frac{1}{\sqrt{2}} \sum_n \{\psi_n(r_2)F_n^{\pm}(r_1) \pm \psi_n(r_1)F_n^{\pm}(r_2)\}$$

where + and — signs correspond to singlet and triplet states respectively and ψ_n represent the wave function for the n-th state of the hydrogen atom and satisfies the eigen value equation

$$(\Delta^2 - 2/r - 2E_n)\psi_n(r) = 0,$$

E_n represents the eigen energy of the n-th state of the atom.

If such functions can be had in which $F^{\pm}_n$ have the asymptotic forms

$$F^{\pm}_n \sim e^{ik_0 r}\delta_{n0} + \frac{e^{ik_n r}}{r} f^{\pm}_n(\theta, \phi)$$

then the respective differential cross sections for excitations of the n-th state for antiparallel and parallel alignment of electrons are

$$\frac{K_n}{K_0} |f^{\pm}_n(\theta, \phi)|^2.$$

Here total energy $E = \frac{K^2_0}{2} + E_0 = \frac{K^2_n}{2} + E_n$ and E_0 represent the eigen energy of the ground state of the atom, K_0, K_n represent respectively the momenta of the incident electron and scattered electron after excitation of the n-th state of the atom.

We shall consider only the symmetric wavefunction corresponding to the singlet case and neglect all states for $n \neq 0$. Henceforth we shall omit the superscript '+' for convenience.

Therefore, $$\psi(r_1, r_2) = \frac{1}{\sqrt{2}} [\psi_0(r_1)F_0(r_2)+\psi_0(r_2)F_0(r_1)] \quad \ldots \quad (2a)$$

with

$$F_0(r) \sim e^{ik_0.r}+ \frac{e^{ik_0r}}{r}f(\theta, \phi) \quad (2b)$$

To solve eqn. (1) under the boundary conditions in (2b), we shall use Hulthén's variational method choosing our trial wave function $\psi(r, r_2)$ as

$$\psi(r_1, r_2) = \chi(r_1, r_2)\, F_0(r_2)+\chi(r_2, r_1)\, F_0(r_1) \quad \ldots \quad (3)$$

where $$\chi(r_1, r_2) = \psi_{1s}(r_1) \left\{ 1- \frac{\alpha^2+\beta^2}{2} \,.\, e^{-2\mu r_2}\right\}$$

$$+\alpha\psi_{2s}(r_1)\,.\, e^{-\mu r_2}+\beta\psi 2p_0(r_1, r_2)e^{-\mu r_2} \quad \ldots \quad (3a)$$

the polar axis being along r_2, $\mu = 1$

and $$F_0(r_2) = \left\{ \frac{\sin K_0r_2}{K_0r_2} +(a+be^{-r_2})(1-e^{-r_2}) \frac{\cos k_0r_2}{K_0r_2}\right\} \quad \ldots \quad (3b)$$

It may be mentioned that we have considered only S-wave scattering and as in our previous work (1965) χ satisfies the normalisation condition $\int \chi^*\chi\, dr_1 = 1$ correct to terms of the order of α^2 and β^2.

Substituting $\psi(r_1, r_2)$ from (3), (3a) and (3b) in the variational integral $L = \int \psi^*(H-E)\psi dr_1\, dr_2$ and using Hulthén's variational method, the value of a is determined, the phase shift is related to a by $\eta_0 = \tan^{-1}a$ neglecting higher powers of α and β.

RESULTS AND DISCUSSIONS

We have evaluated only the singlet S-wave phase-shift values (η_0) for the case $b = 0$ in the trial function $F_0(r_2)$ for energies below the threshold for excitation of second quantum levels by using only the coupling of $1S$, $2S$ and $2P_0$ states.

We have plotted the phase-shifts η_0 against K_0^2 in Fig. 1, where we notice the peculiar resonating behaviour i.e. there is a sharp increase in phase-shift values above $K_0^2 = .70$.

We have shown Q_{res} as a function of K^2_0 in Fig. 2. By making use of Breit-Wigner cross-section formula

$$Q_{res} = \frac{4\pi}{K_0^2} \cdot \frac{\Gamma^2/4}{(E-E_{res})^2+ \frac{\Gamma^2}{4}},$$ we obtain

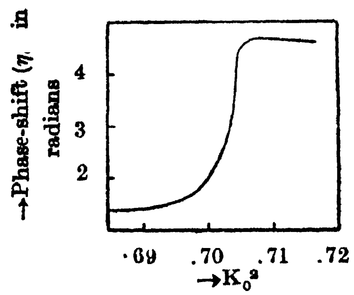

Fig. 1. The singlet S-wave phase shift is plotted as a function of K^2_0 in the neighbourhood of resonance.

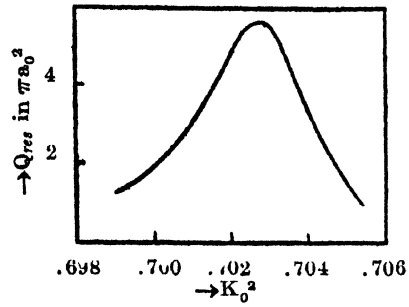

Fig. 2. The resonance part of S-wave cros section is plotted as a function of K^2_0.

$E_{res} = (.7027$ a.u.) 9.55ev, the width $\Gamma \sim .04$ev and the resonance cross section $= 5.56\pi a^2_0$.

The first experimental report on a resonance in the scattering of electrons by atomic hydrogen has been made by Schulz (1964) at (9.7±.15)ev. Such a resonance has been further confirmed by the observations of Kleinpoppen and Raible (1965) who found that it is centred around (9.73±.12)ev. Recently McGowan et. al., (1965) have reported two resonances, one near 9.45ev and the other near 9.68ev.

Burke and Schey (1962) have obtained a rsonance at 9.61ev with a width of .109 ev in the ^1S state and the corresponding resonance cross section being $5.66\pi\ a^2_0$. Nearly similar results were obtained by O'Malley and Geltman (1965), Temkin and Pohle (1965) and others. Most recently, Burke and Taylor (1966) have obtained two resonances, one at 9.560 ev and the other at 10.178 ev with widths of .0475 ev and .00279 ev respectively.

In conclusion, we may say that our present formulation yields satisfactory results for the position of elastic resonance in $\bar{e}$—H scattering.

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